Coarsening of two dimensional XY model with Hamiltonian dynamics: Logarithmically divergent vortex mobility

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We investigate the coarsening kinetics of an XY model defined on a square lattice when the underlying dynamics is governed by energy-conserving Hamiltonian equation of motion. We find that the apparent super-diffusive growth of the length scale can be interpreted as the vortex mobility diverging logarithmically in the size of the vortex-antivortex pair, where the time dependence of the characteristic length scale can be fitted as $L(t) \sim ((t + t_0) \ln(t + t_0))^{1/2}$ with a finite offset time t_0. This interpretation is based on a simple phenomenological model of vortex-antivortex annihilation to explain the growth of the coarsening length scale $L(t)$. The nonequilibrium spin autocorrelation function $A(t)$ and the growing length scale $L(t)$ are related by $A(t) \simeq L^{-\lambda}(t)$ with a distinctive exponent of $\lambda \simeq 2.21$ (for $E = 0.4$) possibly reflecting the strong effect of propagating spin wave modes. We also investigate the nonequilibrium relaxation (NER) of the system under sudden heating of the system from a perfectly ordered state to the regime of quasi-long-range order, which provides a very accurate estimation of the equilibrium correlation exponent $\eta(E)$ for a given energy E. We find that both the equal-time spatial correlation $C_{nr}(r,t)$ and the NER autocorrelation $A_{nr}(t)$ exhibit scaling features consistent with the dynamic exponent of $z_{nr} = 1$.

I. INTRODUCTION

Phase ordering kinetics refers to a study of nonequilibrium dynamic processes of statistical mechanical systems approaching toward the thermal equilibrium of ordered states with broken symmetry. The system is usually quenched from a random disordered state to a low-temperature ordered state below the transition temperature [1, 2]. The ever-nonequilibrium approach to ordered state, in the thermodynamic limit, is usually characterized by the dynamic scaling accompanied by power-law growth of typical length scales of the system. These power law exponents depend on the spatial dimension and the symmetry of the ground states. More importantly these power laws also depend on the nature of the dynamic protocols such as whether the order parameter is conserved or not during the phase ordering processes. Usually, characteristic topological defects, such as point vortices or domain walls, are generated in the initial disordered state, depending on the dimension of the order parameter, and the phase ordering processes can also be interpreted as the process of annihilation and decay of these topological defects: the motion of these defects (and their annihilation) determines the characteristics of the coarsening processes.

Most of the computational works on phase ordering kinetics have been based on a purely dissipative dynamics. In this case, we expect that the motion of the vortices would be also purely dissipative. Energy scaling arguments in combination with conservation laws could determine the growth laws for most of the $O(n)$ spin systems in d dimensions [2] (except for the special case of $d = n = 2$).

In reality, however, there exist various systems exhibiting dynamic processes that cannot be described solely by dissipative dynamics. For example, inertial effects would be present in the case of magnetic spin systems, where the spins are influenced by neighboring spins via precession interaction terms that are energy conserving [3–5] that are often called reversible mode coupling. Actually, among the eight model systems classified by Hohenberg and Halperin [6, 7] for describing the dynamic critical phenomena, five of them (models E, F, G, H, and J) include reversible mode couplings.

We may also take a microcanonical approach to the nonequilirium dynamics by modeling the dynamics of the system based on a purely Hamiltonian dynamics with energy conservation. In relation to this, there have been some research efforts in recent years toward investigating the statistical mechanical behavior of lattice spin systems by solving directly the Hamiltonian equation of motion associated with the spin system [8]. For example, equilibrium phase transitions have been found to be related to a topological change in the dynamics [9–14]. In terms of nonequilibrium phase ordering dynamics, Zheng investigated via Hamiltonian dynamics the coarsening of the Ising-type ϕ^4 model on a two-dimensional square lattice with nonconserved order parameter [15, 16].

In this work, we study numerically the coarsening process of an XY model on a square lattice using Hamiltonian dynamics. This work is built upon a previous preliminary work [17] on the same model system, which we think is incomplete, especially in terms of the analysis on the growth law.

In equilibrium, the XY model exhibits a Berezinskii-Kosterlitz-Thouless (BKT) transition at T_{BKT} due to the

unbinding of vortex-antivortex pairs [18]. Below T_{BKT}, the system has a quasi-ordered phase that is characterized by a power-law decay of the order parameter correlation function for long distances. The critical exponent governing the power-law decay decreases *continuously* down to zero temperature: the system is critical at equilibrium for all non-zero temperatures below T_{BKT}.

The phase ordering dynamics of the XY model has been studied for quite a long time by many groups [19–29]. It is now agreed that, in the phase ordering dynamics of the XY model with non-conserving order parameter (via Monte Carlo simulations or Langevin dynamics methods), the growing length scale $L_{MC}(t)$ exhibits a logarithmic correction [30] to diffusive growth as $L_{MC}(t) \sim (t/\log t)^{1/2}$. Since the coarsening in XY model is dominated by the annihilation of vortex-antivortex pairs generated in the random initial states, we may interpret the growth law in terms of the mobility (or friction) characteristics of the vortices. Here, the logarithmic correction can be attributed to a logarithmic divergence (in the system size) of the effective friction constant of a moving vortex in the dissipative dynamics with a non-conserving order parameter. Another system that can be described by XY model at equilibrium is an array of superconducting Josephson junctions. In the cases of superconducting-normal-superconducting (SNS) junction arrays, the dynamics is often described by resistively-shunted junction (RSJ) model. This model is characterized by a Laplacian type of coupling between time derivatives of superconducting phases of neighboring islands. Due to this particular type of dissipative coupling in Josephson junction arrays, there is *no* logarithmic correction in the growing length scale that corresponds to a finite friction constant of a moving vortex [31].

One further experimental system that can be described by XY model is a thin film of superfluid helium. The dynamics of this system is characterized by a reversible mode-coupling term. In recent simulations on the coarsening dynamics of XY model with reversible mode-coupling (MCXY), it was shown that the growth law exhibits a *positive* logarithmic correction which is opposite to the coarsening of ordinary XY model with purely dissipative dynamics and non-conserving order parameter [5]. This system apparently exhibits a growth law with an exponent that is a little larger than the diffusive growth exponent of $1/2$. But this was re-analyzed and fitted in terms of a (positive) logarithmic correction to a diffusive growth. The growth law could also be understood in terms of a simple vortex-antivortex annihilation model. These features reminded us of the growth law with apparent super-diffusive exponents in the coarsening of XY model with Hamiltonian dynamics [17].

Now, in this work, we perform more extensive simulations on the Hamiltonian coarsening of XY model and carry out an analysis of the growth law in more details in order to determine whether these similarities between MCXY and Hamiltonian XY models are indeed valid.

Due to the Hamiltonian dynamics nature of our system, the total energy is conserved, and we specify the initial states by their total energy divided by the system size, i.e., the per-site energy E. These initial states with specified energies are prepared with a special Monte Carlo algorithm [17]. The initial rotational velocities of the rotors are taken to be zeros, ensuring that the initial configuration is maximally disordered within the constraint of the fixed energy.

Since we begin with zero kinetic energy (zero rotational velocities for all rotors), the Hamiltonian dynamics of the system will generate kinetic energy taken from the potential energy. As time proceeds, we can expect that (for a per-site energy that is low enough to correspond to a low-temperature quasi-ordered phase), the system will evolve toward some equilibrium stationary state which can be considered as corresponding to the ordinary thermal equilibrium state with critical quasi-long-range order. In other words, the kinetic energy that is generated during the course of coarsening process acts as a thermal bath for the system. We investigate the time-dependent spin configuration for the system in terms of spatial ordering and relaxation of the vortex numbers, etc., in analogy to the conventional dissipative coarsening systems.

We find that the equal-time spatial correlation functions satisfy critical dynamic scaling

$$C(r,t) = r^{-\eta(E)}g(r/L(t)), \qquad (1)$$

with a spatial correlation exponent $\eta(E)$ (which is increasing in the per-site energy E) and a growing length scale $L(t)$ that grows typically as $L(t) \sim t^{1/z}$, where z is the dynamic exponent. In the late time region, we find that the length scale $L(t)$ grows with an exponent $1/z$ that is apparently a little larger than the diffusive exponent $1/2$. However, from more detailed analysis we could confirm that the growth of the length scale can be interpreted as the vortex mobility diverging logarithmically in the size of the vortex-antivortex pair. The growth of characteristic length scale can be fitted as $L(t) \sim ((t + t_0)\ln(t + t_0))^{1/2}$ with a finite offset time t_0. This offset time t_0 corresponds to a finite length scale L_0 at $t = 0$ due to the finite average spacing between vortices and antivortices at the initial time.

We could also compare the nonequilibrium spin autocorrelation function $A(t)$ of the order parameter in the coarsening process and the growing length scale $L(t)$. Here, we found that $A(t)$ and the $L(t)$ are related by a scaling exponent λ with $A(t) \simeq L^{-\lambda}(t)$ where $\lambda \simeq 2.21$ (at $E = 0.4$) with only very weak monotonic increase on the value of E. This is rather close to that in the case of MCXY or (soft-spin) model E [5]. While, on the other hand, this value of λ exponent is quite different from that of usual dissipative coarsening dynamics of XY model (or $O(2)$ model) with nonconserved order parameter where the exponent of $\lambda \sim 1.17$ was predicted theoretically and also observed in numerical simulations [25, 32–35]. This implies that the system loses its memory much more quickly in the Hamiltonian dynamics or in

the case of MCXY than in the case of simple dissipative dynamics.

Our simulation results indicate that the phase ordering kinetics of Hamiltonian XY model belongs to the same universality class as that of the Langevin dynamics of XY model with a reversible mode-coupling and also that of (soft-spin) model E dynamics. This seems to be due to the existence of the same symmetry and conservation law in the two systems. That is, the total rotational momentum is conserved in the Hamiltonian dynamics which corresponds to the conservation of the third component (or the conjugate momentum) in the model E dynamics. Due to the conservation of the rotational momentum, propagating spin wave modes appear [36, 37]. This propagating spin wave modes might interact with the vortices and antivortices such that the mobility diverges logarithmically as the distance between vortices and antivortices increases. As in the previous work on the phase ordering dynamics of MCXY model, here also we attempt to fit the growth of the length scale with a simple phenomenological dynamic model of coarsening based on vortex-antivortex annihilation.

In order to analyze the critical dynamic scaling of the equal-time spatial correlation of the order parameter, we need an accurate estimate of the spatial correlation exponent $\eta(E)$. For accurate measurement of $\eta(E)$, we employ an analog of the so-called nonequilibrium relaxation (NER) method. Here one starts with a perfectly ordered initial state but with random finite rotational velocities such that the total kinetic energy per site is equal to E. Beginning with this initial state, the system evolves toward a steady dynamic state corresponding to a critical equilibrium state. By analyzing the approach to the steady state in terms of the equal-time spatial correlation function of the order parameter, we can estimate more accurately the equilibrium correlation exponent $\eta(E)$. In this case of NER relaxation, we can also obtain approximate analytic expression for the equal-time spatial correlation and autocorrelation function by using spin-wave approximation (see APPENDIX A), which agrees qualitatively well with simulation results.

II. THE HAMILTONIAN XY MODEL AND SIMULATION METHODS

The dynamic equation of the hard-spin XY model on a square lattice (of linear size N) can be obtained from the following Hamiltonian given by

$$H = \frac{1}{2}\sum_i m_i^2 + J \sum_{<ij>} \Big[1 - \cos(\theta_i - \theta_j) \Big], \qquad (2)$$

where, J is the interaction strength, θ_i is the phase angle of the spins at site i and the sum is over nearest neighbor pairs. In the kinetic term, $m_i = \dot{\theta}_i$ represents the

angular momentum associated with the angular variable θ_i of planar spin at site i. This model appears naturally in easy-plane ferromagnets or superfluid helium with the conserved variable m corresponding to the z-component of the spin or the density of the superfluid in the limit of negligible thermal noise (e.g., negligible phonon effect) [4, 6].

Previous works [11, 12] have shown that a BKT transition occurs at the value of the per-site energy around $E_{BKT} \simeq 1.0$. In this work, we perform simulations of Newtonian dynamics based on the above Hamiltonian with initial states of zero kinetic energy and a pre-specified potential energy E (but otherwise with random initial phases). Specified potential energy values are chosen from the region that corresponds to below the BKT transition energy ($E_{BKT} \simeq 1.0$).

Unlike the case of dissipative systems with Langevin dynamics or Monte Carlo dynamics where dissipative relaxation is incorporated in a natural way, here in our case of Hamiltonian dynamics, the total energy (sum of kinetic and potential energy) is conserved. However, since we begin the Hamiltonian dynamics with zero kinetic energy with a given specified maximal potential energy, we expect that the system will evolve in such a way as to decrease (on the average) the potential energy and increase the kinetic energy. Eventually, in the long-time limit, the system will reach a certain kind of near-equilibrium dynamic state where the average potential energy and the kinetic energy do not vary appreciably. Of course, rigorously speaking, in the thermodynamic limit, the system will never reach a complete equilibrium state in a finite time period.

Therefore, we can consider the kinetic part of the system acting as a kind of thermal heat bath that absorbs the "dissipated heat" coming from the decreasing potential energy. We can, thus, investigate the time-dependent spin configurations for the system in terms of spatial ordering and relaxation of vortex numbers, etc. We generate the initial states with specified potential energies in the following manner. To begin with, we take a random spin configuration. Then we employ a Monte Carlo annealing algorithm such that the spin configurations with potential energies that are closer to the target energy are preferentially accepted. In other words, we steer the initial state to some target spin configuration such that we obtain a state whose potential energy is equal to a specific energy. In other respects (i.e., except for the constraint of the specified energy), the spin configuration is kept random.

The Hamiltonian equation for Eq. (2) reads

$$\dot{m}_i = -\frac{\partial U}{\partial \theta_i} = -J \sum_j \sin(\theta_i - \theta_j), \qquad (3)$$

$$\dot{\theta}_i = m_i \qquad (4)$$

where j denotes the nearest neighbors of site i with $i = 1, \cdots, N^2$. For simplicity, we set the rotational inertia to be equal to unity and put $J = 1$. Here, we

note that, in addition to the conservation of total energy, another conserved quantity exists, namely the total rotational momentum $\sum_i m_i \equiv \sum_i \dot{\theta}_i$. This is due to the invariance of the equations under global rotations in the variable θ_i, that is, under $\theta_i \rightarrow \theta_i + \alpha$.

Equations (2) and (3) are numerically integrated in time using a second order velocity-Verlet algorithm [38] with the time integration step of $\Delta t = 0.01$, which conserves the total energy to within a ratio of 10^{-4} up to the maximal time integration steps of around 10^6. Periodic boundary conditions on both lattice directions are employed. The simulations are carried out on square lattices of dimensions up to $N \times N = 2000 \times 2000$ with sample averages of over 40 to 150 different initial configurations. A parallel computation is employed via a domain decomposition method with high parallel efficiency.

The main quantities of interest are as follows:

(i) Equal-time spatial correlation function of the order parameter,

$$C(r,t) = \frac{1}{N^2} \left\langle \sum_i \cos(\theta_i(t) - \theta_{i+r}(t)) \right\rangle, \qquad (5)$$

where $< \cdots >$ denotes an average over random initial configurations.

(ii) The total number of vortices and antivortices $N_V(t)$ at time t, and

(iii) Nonequilibrium spin autocorrelation function

$$A(t) \equiv \frac{1}{N^2} \left\langle \sum_i \cos(\theta_i(0) - \theta_i(t)) \right\rangle. \qquad (6)$$

III.   SIMULATION RESULTS AND DISCUSSIONS

A.   Nonequilibrium relaxation (NER) from fully ordered state

As was mentioned in the introduction, the equal-time spatial correlation function in the coarsening process is expected to obey a critical dynamic scaling (Eq. (1)). One of the parameters to be determined is the equilibrium correlation exponent $\eta(E)$. We may try to fit the equal-time spatial correlation function for the coarsening dynamics with $\eta(E)$ as a free parameter. In this case, various values of $\eta(E)$ should be chosen on a trial and error basis, and the best dynamic scaling collapse must be chosen among these many possibilities. This is not a very accurate or reliable procedure let alone being tedious.

Instead, we have a better way to estimate the values of $\eta(E)$ independently. This is the so-called NER method

where, in the usual case, the system is instatntaneously brought from a perfectly ordered state to a finite temperature T. This target temperature is usually chosen as the critical temperature corresponding to a second order phase transition. Here, in our case of Hamiltonian dynamics, the energy per site E is conserved. It is easy to see that an analog of NER method here can be achieved as follows. Similar to the case of usual lattice spin system under thermal noise, here, one starts with a perfectly ordered initial state. But we have to remember that the per-site energy of the system has to be conserved (equal to E). Since the perfectly ordered initial state has zero potential energy (from our definition of the Hamiltonian in Eq. (2)), the rotational velocities $\dot{\theta}_i$ in the initial configuration should be chosen such that the initial per-site kinetic energy be equal to E. Except for this constraint of energy conservation, the initial velocities are chosen randomly. Beginning with this initial state of perfect order but with finite kinetic energy (through random rotational velocities), when the initial kinetic energy per site is low enough, the system will evolve toward a steady state corresponding to a critical equilibrium state at a finite temperature (correspondng to temperatures below the BKT transition).

By analyzing the approach to the steady state in terms of the equal-time spatial correlation function of the order parameter, we can compute more accurately the equilibrium correlation exponent $\eta(E)$. The NER equal-time spatial correlations for the case of $E = 0.4$ are shown in Fig. 1a. As time elapses, spatial extent of critical power law relaxation increases with a clear power exponent. In order to extract the η exponent more rigorously, we analyze the data with a critical dynamic scaling

$$C_{nr}(r,t) = r^{-\eta(E)} g_{nr}(r/L_{nr}(t)), \qquad (7)$$

with the spatial correlation exponent $\eta(E)$ and a growing correlation length scale $L_{nr}(t)$ with $L_{nr}(t) \sim t^{1/z_{nr}}$. A good collapse of the rescaled correlation functions is shown in Fig. 1b. Interestingly, we find that the correlation length scale $L_{nr}(t)$ exhibits a linear growth in time as $L_{nr}(t) \sim t$ i.e., $1/z_{nr} \simeq 1$ which is quite different from the case of nonconserved dissipative dynamics where the diffusive exponent $1/2$ is observed [39]. This may be attributed to the effect of propagating spin wave mode in the linearized equation of motion. Indeed, in the spin-wave approximation, we find that the equal-time spatial correlation $C_{nr}(r,t)$ can be expressed in closed form (see the Appendix A) which exhibits critical dynamic scaling and linear growth of the length scale $L_{nr}(t)$ with

$$C_{nr:SW}(r,t) \simeq r^{-\eta_{SW}(E)} g_{nr:SW}(r/2t)) \qquad (8)$$

where $\eta_{SW}(E) = E/2\pi$ and

$$g_{nr:SW}(u) = u^{\eta_{SW}(E)} \left(\frac{1 + \sqrt{1-u^2}}{1 - \sqrt{1-u^2}} \right)^{\eta_{SW}(E)/2} \qquad (u < 1),$$

$$= u^{\eta_{SW}(E)} \quad (u > 1). \qquad (9)$$

where SW in the subscript refers to "spin-wave approximation". The behavior of $C_{nr}(r,t)$ vs. r at the latest time $t = 320$ in simulation for several cases of the energy E are shown in Fig. 1c with the $\eta(E)$ exponents and the spin-wave approximation values $\eta_{SW}(E)$ in the inset. We can see an approximate agreement between the simulation results of $\eta(E)$ and $\eta_{SW}(E)$ especially at low E which is consistent with the spin-wave approximation. If we consider the case of $E = 0.4$, the simulation results of $\eta(E = 0.4) = 0.071$ can be compared reasonably with the approximate analytic value of $\eta_{SW}(E) = E/2\pi \simeq 0.064$ at spin-wave approximation. Also, with the same approximation, we could easily derive the formula for the auto-correlation $A_{nr:SW}(t)$ as $A_{nr:SW}(t) \sim t^{-\eta_{SW}(E)/2}$ (see APPENDIX A).

B. Critical coarsening dynamics

Now we turn to the critical coarsening dynamics evolving from random configurations. Figure 2a shows the equal-time spatial correlations for $E = 0.4$ for different time instants. We attempt a critical dynamic scaling

$$C(r,t) = r^{-\eta(E)} g(r/L(t)), \qquad (10)$$

where we use the spatial correlation exponent $\eta(E)$ obtained from the NER analysis shown above. In our case, for a given time instant t, we determined $L(t)$ in such a way that $r^{\eta(E)} C(r,t)|_{(r=L(t))} = g(r/L(t))|_{(r=L(t))} = g(1) = 0.4$. Shown in Fig. 2b is such an attempt at critical dynamic scaling where we find that the equal-time spatial correlation functions exhibit a reasonable critical dynamic scaling, at least, in the late-time regime.

In the late-time regime, we find that the length scale $L(t)$ grows with an effective exponent $1/z$ that is apparently larger than the diffusive exponent 0.5. For example, in the case of $E = 0.4$, we obtain $1/z \simeq 0.553 \pm 0.005$, which is a little larger than $1/2$ (Fig. 2c). This is consistent with the previous work [17]. In contrast, in the conventional purely diffusive case, the effective growth exponents obtained numerically are invariably smaller than $1/2$ due to a negative logarithmic correction. Similar enhancement of growth was observed recently in the coarsening dynamics of the (soft spin) model E as well as the MCXY model. There, it was interpreted as the result of a logarithmically divergent mobility of vortices (and antivortices) in terms of a simplified kinetic model of a single pair of vortex and antivortex. Here we find that the same model can explain the coarsening process only with a modification of the initial condition that accounts for the finite length scale L_0 at time $t = 0$ due to the special nature of Hamiltonian dynamics and corresponding energy conservation in the present system. Similar phenomenon of logarithmically divergent mobility was also found experimentally in the quasi-two-dimensional diffusion of colloids [40] or diffusion of protein molecules on the membranes [41] under hydrodynamic effect, and also in numerical simulations of the vortex diffusion in the anisotropic Heisenberg system in two dimensions with spin precession [42–44].

We reiterate briefly on the single vortex-antivortex annihilation model. We can see that, in order for the system to reach a state with average length scale of R, vortex pairs of sizes on the order of R must be already annihilated. Ignoring the very complicated many-body process involving many vortex pairs during this process, we simplify the whole coarsening process (corresponding to the growth of the length scale up to R) by the annihilation of *single* vortex-antivortex pair of size R with a suitably defined interaction potential.

We assume that the vortex acts like a small particle with finite 'mass' moving under the influence of an external force with a mobility that depends logarithmically on the length scale of the system. Then the distance R between a vortex and an anti-vortex would be described by the following equation of motion

$$m(R)\frac{d^2 R}{dt^2} + \frac{1}{\mu(R)}\frac{dR}{dt} = F(R) = -\frac{k}{R}. \qquad (11)$$

Here, the length-dependent effective mass of a vortex is denoted as $m(R)$ and the length-dependent mobility of a vortex as $\mu(R)$. We also assume that the vortex-antivortex pair is interacting via a Coulombic force $F(R) = -k/R$ in two dimensions. We will set the proportionality constant k as $k = 1$. As for the functional form of the $m(R)$ and $\mu(R)$, we use the same forms as that employed in [5] where logarithmic dependences of the vortex mobility $\mu(R)$ and $m(R)$ are used [42–44] as follows

$$m(R) = m_0 + m_1 \ln(R/r_0), \qquad \mu(R) = \mu_0 + \mu_1 \ln(R/r_0) \qquad (12)$$

where m_0, m_1, μ_0, μ_1 are constants and r_0 denotes a shortest cutoff length scale in the system (corresponding to the vortex core size). Note that m_0 corresponds to the effective mass at the shortest cutoff length scale and similarly for μ_0 for the vortex mobility.

The growth law is obtained by calculating (through integration of the above model dynamic equation) the time τ it takes for a vortex-antivortex pair of size $R = R^*$ to reach a state with $R = R_0$ where R_0 denotes the initial (coarsening) length scale of the system (the average separation between vortices or antivortices). We set the value of dR/dt at $R = R^*$ to be zero. We numerically solve the model equation of vortex-antivortex pair dynamics, Eqs. (11) and (12), to obtain the time τ when the size of the vortex-antivortex pair R becomes equal to R_0. Note that R_0 is larger than the lower cutoff length scale of r_0 corresponding to the unit lattice spacing. By plotting the resulting relation R^* and τ we get the growth law of the coarsening dynamics.

If we assume that the inertial effect is negligible, then, due to the logarithmic divergence of the vortex mobility, we can analytically get the dominant asymptotic growth law as

$$L(t) \sim \left(t\ln t\right)^{1/2}. \qquad (13)$$

However, we note that, in the limit of $t \to 0$, the domain length scale L_0 obtained from our simulations of our Hamiltonian XY model approaches a finite value which is incompatible with the above form (which gives $L(t = 0) = 0$). In order to reconcile with this limiting conditions, we should take a more general ansatz equation for the time dependence of the length scale that exhibits a finite initial value for the length scale and still satisfies the dynamic equation of motion asymptotically. One plausible candidate is the following form which is obtained by a simple shift of the time variable t as

$$L(t) \sim \left((t + t_0) \ln(t + t_0)\right)^{1/2}. \qquad (14)$$

We might also take another form by adding a constant L_0 to Eq. (13) as $L(t) \sim L_0 + a(t \ln t)^{1/2}$. But here we chose the above method of shifting the time because it appears the most natural, being analytic at $t = 0$. We find that $L(t)$ vs. t can be fitted by Eq. (14) in the late time regime (Fig. 2c).

In addition, shown in Fig. 3a is the relaxation of the vortex number density $\rho_v(t)$ for $E = 0.4$. It exhibits a power law relaxation with $\rho_v(t) \sim t^{-1.076}$. If we assume that the vortices are uniformly (and randomly) distributed in two dimensional space, then using a naive argument, we would expect that $\rho_v(t) \sim L^{-2}(t)$. Interestingly, however, we find that the following nontrivial scaling relation holds in the late time region (Fig. 3b)

$$\rho_v(t) \sim L^{-x}(t), \qquad x = 1.93 \qquad (15)$$

This feature is also very similar to the behavior of MCXY model and also that of the model E [5]. We note that the exponent x showed little systematic variation at different values of E except for some statistical numerical fluctuations (data not shown).

The nonequilibrium spin autocorrelation function $A(t)$ is expected to be related to the growing length scale $L(t)$ through a new non-equilibrium exponent λ as

$$A(t) \sim L^{-\lambda}(t). \qquad (16)$$

We could extract the value of λ by plotting $A(t)$ versus $L(t)$ as shown in the Fig. 4, where we can see that, in the long time limit the value of λ approaches $\lambda \simeq 2.21$ for the case of $E = 0.4$. This value is rather close to the value in Ref. [5] (where $\lambda \simeq 1.99$ was observed) but much larger than the value of $\lambda \simeq 1.17$ for the case of non-conserved $O(2)$ model with no reversible mode coupling [25, 32–35]. It was argued in Ref. [5] that the higher mobility of the vortices in the present model causes a faster memory loss of the initial configuration and hence larger value of the λ exponent. It would be interesting if one can find some analytic argument for the value of $\lambda = 2.21$. It appears that, due to the existence of propagating spin wave modes, the spin configuration loses its memory more quickly than in the case of purely dissipative dynamics. We also found that there exists a very weak monotonic increase of the λ exponent with the increase of E [39], which probably is related to the increasing spatial critical exponent $\eta(E)$ at finite temperature. This trend is also consistent with the small difference between the value of λ exponent in the present work and that of MCXY or model E in Ref. [5], since, in the latter case, they are dealing with a zero temperature coarsening. Figure 5 shows a fitting of the full simulation results by our vortex-antivortex annihilation model via integration of Eq. (11) with a suitable choice of the parameters.

We note again that, in our Hamiltonian dynamics simulations, the initial states are not completely random states due to the finite energy constraint, Therefore, the initial states already have some finite correlation length scale, i.e., separation R_0 between vortices. These length scales are of the order of 3 to 5 lattice constants. Therefore, we expect that a finite time scale τ_0 (corresponding to the time scale for a vortex to travel the distance R_0) exists after which a scaling region emerges. It is interesting to note that the effect of the vortex inertia is observed to be not very significant at least for the domain growth law. This might be due to the finite initial length scale L_0. This should be contrasted to the case of the domain growth in the $O(2)$ Ginzburg Landau model with reversible mode coupling. The typical length scale $L_v(t = 0)$ between vortices at initial time can be derived from the number density of vortices, which can be compared with the corresponding length scale L_0 derived from the equal-time spatial correlation functions. We expect that these two length scales are approximately proportional to each other, which is indeed what we found from our data [39]. Note that L_0 was obtained by the arbitrary choice of 0.4 for the value of the cut in the dynamic scaling collapse of the equal-time spatial correlation functions. Since $L_v(t = 0)$ represents the initial average separation between vortices and antivortices at which the value of the rescaled correlation function would most probably be smaller than 0.4, we expect that $L_v(t = 0)$ is larger than L_0. We could also confirm this from the data (data not shown here).

IV. SUMMARY

We have studied the coarsening dynamics of the Hamiltonian XY model on two-dimensional square lattice. An initial state that is specially tuned to have a given potential energy (otherwise random) but with zero kinetic energy develops into a late-time coarsening state, where the potential energy slowly decays as a power law with a compensating increase in the kinetic energy. In order to compute accurately the equilibrium correlation exponents $\eta(E)$ for the order parameter, we employed an analog of the so-called NER method where the system begins with a perfect order but with finite kinetic energy. An interesting scaling behavior emerged here with linear growth of the nonequilibrium correlation length. In the coarsening dynamics, the growth of the characteristic length scale can be fitted as $L(t) \sim ((t + t_0) \ln(t + t_0))^{1/2}$

with a finite offset time t_0 which is due to the existence of a finite separation between vortices and antivortices at the initial time. The growth of the length scale can be interpreted as the vortex mobility diverging logarithmically in the size of the vortex-antivortex pair. A simple phenomenological dynamic model of vortex-antivortex annihilation can fit the growth of the length scale, with a suitable set of parameters for the effective inertia and mobility of vortices that are dependent on the growing length scale. The nonequilibrium spin autocorrelation function $A(t)$ and the $L(t)$ are related through the nonequilibrium exponent λ by $A(t) \simeq L^{-\lambda}(t)$ with an exponent of $\lambda \simeq 2.21$ (at $E = 0.4$) which is distinctly different from the case of ordinary $O(2)$ or XY model with dissipative dynamics.

Appendix A: Critical dynamic scaling of the correlation functions in spin-wave approximation

Here we analytically show that the critical dynamic scaling Eq. (7) holds in the spin-wave approximation. We consider the equation of motion for the spin-angle variables θ_i. For convenience of notation, we denote here θ_i as $\theta(\mathbf{r}, t)$ at position $\mathbf{r}$ (instead of i) and time t. In the spin-wave approximation with continuum notation, the Hamiltonian equation of motion reads as follows

$$\frac{\partial^2 \theta(\vec{r}, t)}{\partial t^2} - \nabla^2 \theta(\vec{r}, t) = 0 \tag{A1}$$

which is the same as a wave equation. Here we simply put the wave velocity $c \equiv 1$. We want to calculate the equal-time spatial correlation of the spins for the case of perfectly ordered initial spin configuration (but with finite angular velocities) which is defined as

$$C_{nr}(r, t) = \langle \exp\left[i\theta(\mathbf{r}, t) - i\theta(\mathbf{0}, t)\right] \rangle, \tag{A2}$$

and the nonequilibrium spin autocorrelation function

$$A_{nr}(t) \equiv \langle \exp\left[i\theta(\mathbf{r}, t) - i\theta(\mathbf{r}, 0)\right] \rangle. \tag{A3}$$

General solutions for the wave equation can be written as

$$\theta(\mathbf{r}, t) = \int_{\mathbf{k}} \left(f_{\mathbf{k}}^+ \exp(i\mathbf{k} \cdot \mathbf{r} + i\omega t) + f_{\mathbf{k}}^- \exp(i\mathbf{k} \cdot \mathbf{r} - i\omega t) \right) \tag{A4}$$

where $\int_{\mathbf{k}} \equiv \int d^2k/(2\pi)^2$ and $\omega = |\mathbf{k}| = k$. With the initial condition of $\theta(\mathbf{r}, t = 0) = 0$, we get $f_{\mathbf{k}}^+ = -f_{\mathbf{k}}^- \equiv f_{\mathbf{k}}/2i$ with

$$\theta(\mathbf{r}, t) = \int_{\mathbf{k}} f_{\mathbf{k}} \exp(i\mathbf{k} \cdot \mathbf{r}) \sin(\omega t). \tag{A5}$$

We assume that the initial angular velocity at each site has a Gaussian distribution with zero mean and standard deviation proportional to the square root of the average energy per site. In addition, it is also assumed that the angular velocities exhibit delta-function correlations between different spatial points. If the average energy per site is given by E, then we have $\left\langle \dot{\theta}(\mathbf{r}, 0) \dot{\theta}(\mathbf{r}', 0) \right\rangle = 2E\delta(\mathbf{r} - \mathbf{r}')$, which, in the wave-vector space, can be written as

$$\langle f_{\mathbf{k}}\, f_{\mathbf{k}'} \rangle = \frac{8\pi^2 E}{k^2} \delta(\mathbf{k} + \mathbf{k}'). \tag{A6}$$

Combining above relations and also using the gaussian nature, we can obtain the following

$$C_{nr:SW}(r, t) = \exp\left[-\frac{1}{2}\left\langle (\theta(\mathbf{r}, t) - \theta(\mathbf{0}, t))^2 \right\rangle\right]$$
$$= \exp\left[-\frac{E}{\pi^2}\int d^2k\, \frac{1}{k^2} \sin^2\left(\frac{1}{2}\mathbf{k} \cdot \mathbf{r}\right) \sin^2(kt)\right]. \tag{A7}$$

In order to compute the integral inside the exponential, we put

$$J(\vec{r}, t) \equiv \int d^2k\, \frac{1}{k^2} \sin^2\left(\frac{1}{2}\mathbf{k} \cdot \mathbf{r}\right) \sin^2(kt) \tag{A8}$$

Taking a derivative of J with respect to t and also adding prescription for the proper convergence in the (positive) large k limit, we arrive at

$$\frac{\partial J(r, t)}{\partial t} = \lim_{\epsilon \to +0} \frac{1}{2} \int_0^{2\pi} d\phi \int_0^\infty dk \sin(2kt) \times \left(1 - \cos\left(k\, r \cos\phi\right)\right) \exp(-\epsilon k). \tag{A9}$$

This integral can now be easily done with the following result

$$\frac{\partial J(r, t)}{\partial t} = \frac{\pi}{2t}\left(1 - \left[1 - (r/2t)^2\right]^{-1/2}\right) \quad (\frac{r}{2t} < 1),$$
$$= \frac{\pi}{2t} \quad (\frac{r}{2t} > 1). \tag{A10}$$

The above equation can now be integrated with respect to t with proper boundary conditions, leading to the equal-time spatial correlation function as

$$C_{nr:SW}(r, t) \simeq r^{-\eta_{SW}(E)} g_{nr:SW}(r/2t) \tag{A11}$$

where $\eta_{SW}(E) = E/2\pi$ and

$$g_{nr:SW}(u) = u^{\eta_{SW}(E)} \left(\frac{1 + \sqrt{1-u^2}}{1 - \sqrt{1-u^2}} \right)^{\eta_{SW}(E)/2} \quad (u < 1),$$

$$= u^{\eta_{SW}(E)} \quad (u > 1). \tag{A12}$$

In the limit of $u \equiv r/2t << 1$, we get $C_{nr:SW}(r,t) \sim r^{-\eta_{SW}(E)}(1 - \eta_{SW}(E)u^2/8)$ and also in the other regime of $u \equiv r/2t > 1$, we get $C_{nr:SW}(r,t) \sim t^{-\eta_{SW}(E)}$ independent of the value of r. This agrees qualitatively

with the simulation results including the plateau behavior in the region of $u \equiv r/2t > 1$. The value of $\eta_{SW}(E)$ at spin-wave approximation for $E = 0.4$ is given by $E/2\pi \simeq 0.064$ which is in approximate agreement with the simulation result of $\eta(E = 0.4) = 0.071$ (see Fig. 1c). Also we find for the autocorrelation $A_{nr:SW}(t)$

$$A_{nr:SW}(t) \simeq t^{-\eta_{SW}(E)/2} \tag{A13}$$

which again shows approximate agreement with simulations results (data not shown).

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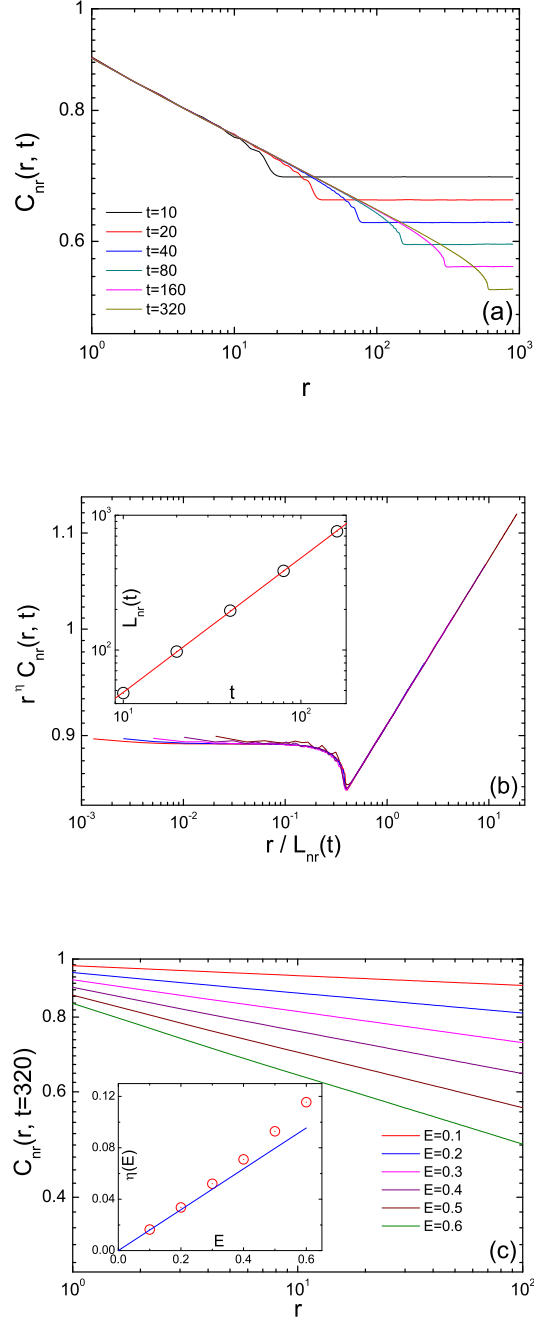
FIG. 1: (a) The equal-time spatial correlation function of the XY spin order parameter with NER dynamics for $E = 0.4$ at times $t = 10, 20, 40, 80, 160, 320$, where the system size is 1800×1800. (b) The scaling collapse of the data in (a) with the appropriate scaling length $L_{nr}(t)$. The inset shows the length scale $L_{nr}(t)$ vs. t which exhibits a linear growth $L_{nr}(t) \sim t^{1/z}$ with $1/z \simeq 1$ and $\eta \simeq 0.071$. (c) The equal-time spatial correlations $C_{nr}(r, t)$ at late time $t = 320$ for different energies. The inset shows the corresponding $\eta(E)$ (circles) and the spin-wave approximation values $\eta_{SW}(E)$ (solid line) versus E.
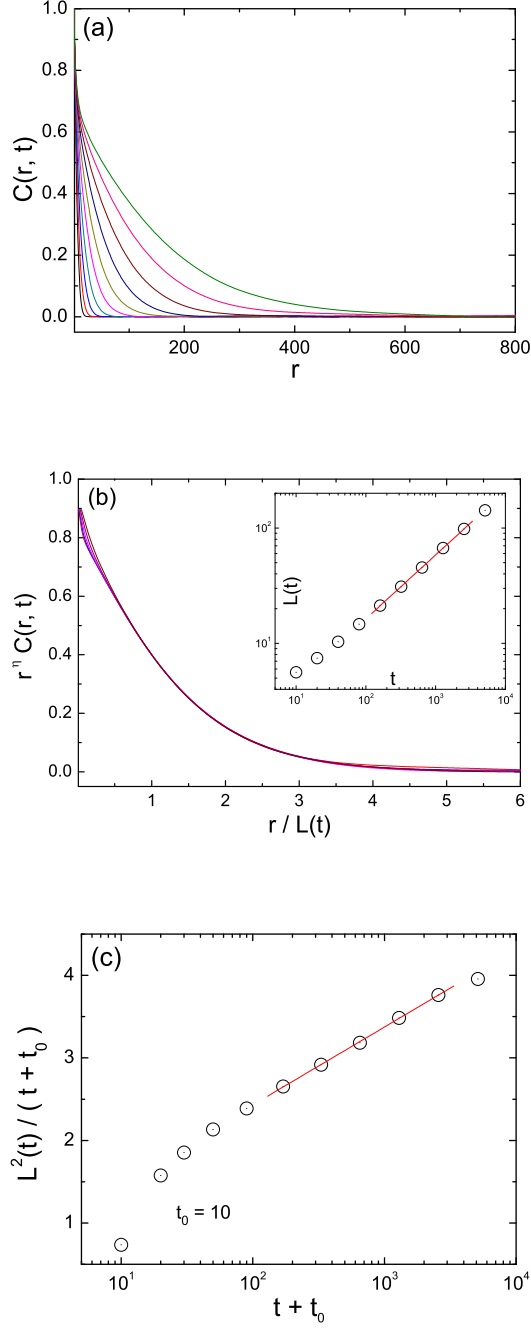
FIG. 2: (a) The equal-time spatial correlation function of the XY spin order parameter with coarsening dynamics for $E = 0.4$ at various times from $t = 10$ up to 5120 with the system size is 2000×2000. (b) The scaling collapse of the data in (a) with the appropriate scaling length $L(t)$ for $t = 160$, 320, 640, 1280 and 2560. The inset shows the length scale $L(t)$ vs. t which exhibits an effective superdiffusive power law growth of $L(t) \sim t^{1/z}$ with $1/z \simeq 0.553$. (c) $L^2(t)/(t + t_0)$ vs. $\ln(t + t_0)$ which indicates a positive logarithmic correction for the growing length scale.
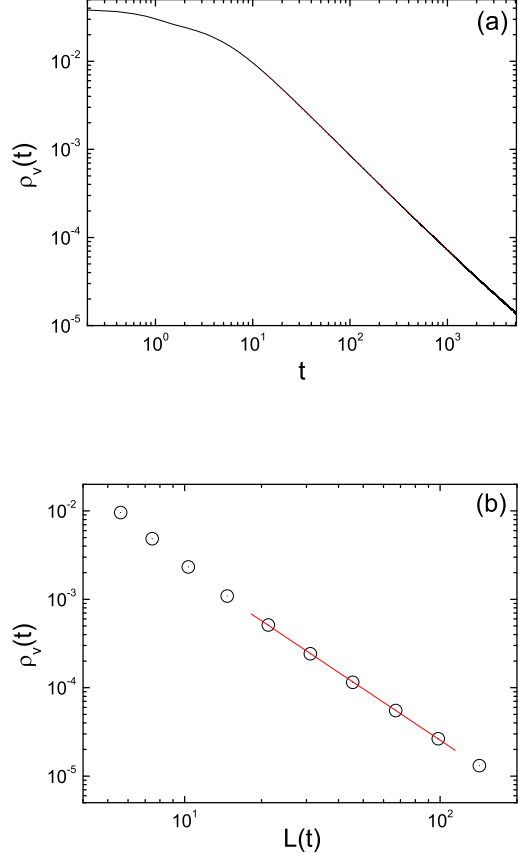
FIG. 3: Relaxation of (a) the vortex number density $\rho_v(t)$ at energy $E = 0.4$ and system size 2000×2000 which shows a power law decay with $\rho_v(t) \sim t^{-1.076}$ (in the time interval between $t = 10$ and 1000). (b) The vortex number density $\rho_v(t)$ vs. $L(t)$ exhibits a power law decay $\rho_v(t) \sim L^{-x}(t)$ with $x \simeq 1.93$.
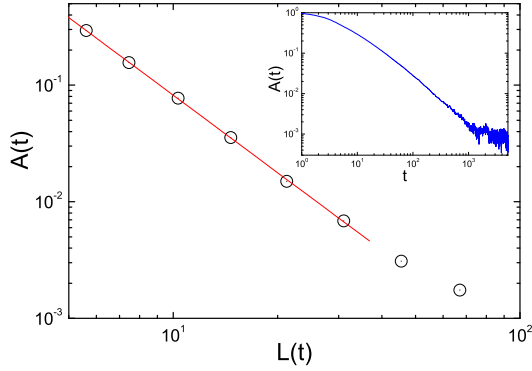

FIG. 4: Spin autocorrelation function vs. $L(t)$ at energy $E = 0.4$ indicating a simple power law relationship between the two with $A(t) \sim L(t)^{-2.21}$.
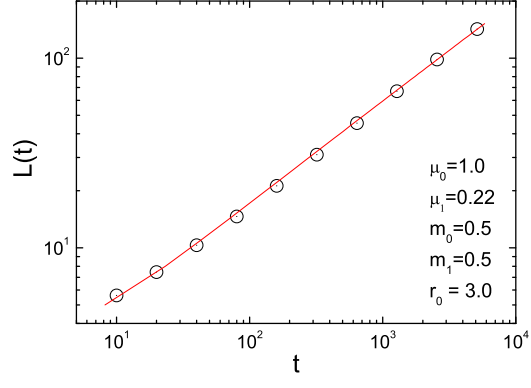
FIG. 5: The growth of $L(t)$ fitted by a simple vortex-antivortex annihilation model at energy $E = 0.4$ which shows a good agreement.